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KEELE UNIVERSITY

EXAMINATIONS, 2010/11

Level III

Tuesday 10^{th} May 2011, 16.00-18.00

PHYSICS/ASTROPHYSICS

PHY-30009

QUANTUM PHYSICS OF ATOMS AND MOLECULES

Candidates should attempt to answer THREE questions.

NOT TO BE REMOVED FROM THE EXAMINATION HALL

1. A particle of mass m is confined to a ring of radius R. The ene
eigenfunctions for this potential are

$$\psi(\theta) = \sqrt{\frac{1}{2\pi}}\, e^{in\theta}$$

where $n = 0, \pm 1, \pm 2, \ldots$ is any integer. The energies of the states are

$$E_n = \frac{n^2\hbar^2}{2mR^2}.$$

(a) At time $t = 0$ the particle has equal probability of being at all positions within one half of the ring.

i. Show that the wavefunction at time $t = 0$ can be written as

$$\Psi(\theta, 0) = \begin{cases} \frac{1}{\sqrt{\pi}} & 0 \le \theta < \pi \\ 0 & \pi \le \theta < 2\pi \end{cases}$$

[20]

ii. Calculate the probability of observing the particle in the ground state at time $t > 0$. [40]

(b) State and explain the value of the degeneracy of the ground state and first excited state in the case of an electron confined to a ring. [20]

(c) State and explain the boundary conditions that apply to the energy eigenfunctions in this case. [20]

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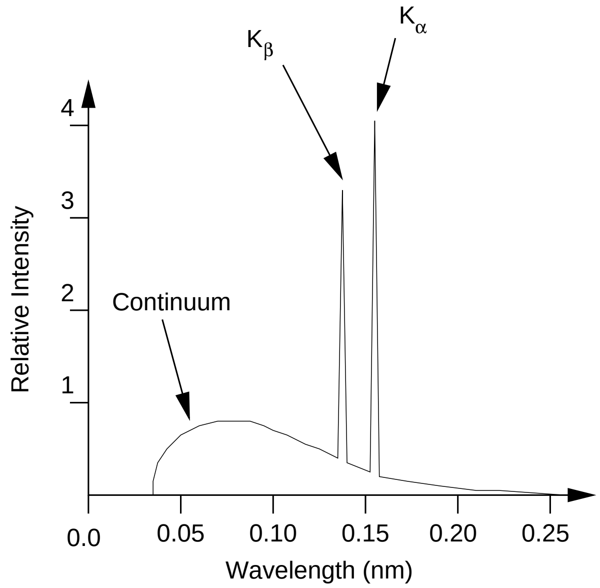
2. (a) The figure below shows the spectrum of X-rays emitted fro sample of copper when bombarded by high energy electrons.



i. Describe the physical origin of the continuum, K_α and K_β features. Explain why this leads to line emission for the K_α and K_β features but a continuous range of wavelengths for the continuum. [20]

ii. Show that the K_α line appears at the wavelength expected given your answer to part i. State clearly any assumptions or approximations used in your calculation. [20]

iii. Estimate the voltage used to accelerate the incident electrons. Explain your method clearly. [15]

(b) Describe with the aid of a sketch the appearance and physical origin of the K-edge and L-edge features in the X-ray absorption spectrum of metals. [25]

(c) Explain briefly how the K-edge feature in the X-ray absorption spectrum of metals can be utilized to examine the composition and structure of mineral samples. [20]

$$[\ E_R = 13.61\,\text{eV}\ ]$$

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3. Barium atoms have two optically active electrons. In the ground state these electrons have the configuration $6s^2$. In one possible excited state these electrons have the configuration $6s^1\,5d^1$.

   (a) Sketch the energy levels for the electrons in both the $6s^2$ and $6s^1\,5d^1$ states using spectroscopic notation to label each state. Your sketch should indicate the correct ordering of the energy levels according to Hund's rules and the relative spacing of different levels. You do not need to provide an energy scale for your sketch. [25]

   (b) Explain why the $6s^1\,5d^1$ state has a higher energy than the $6s^2$ ground state despite one electron having a lower principal quantum number. [25]

   (c) State the transition rules that govern allowed transitions from the $6s^1\,5d^1$ state. Hence, list the transitions that are not forbidden from the $6s^1\,5d^1$ state to the $^3F_{2,3,4}$ triplet of the $6s^1\,5f^1$ state [20]

   (d) For each of the $6s^1\,5d^1$ energy levels, calculate the number of components into which the level is split by a weak magnetic field and state whether the splitting is due to the normal or anomalous Zeeman effect. [15]

   (e) It is observed that for states with the same total spin angular momentum but different values of the total orbital angular momentum, L^T, states with larger L^T values have lower energy. Give a simple physical explanation for this observation. [15]

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4. The rotational energy of a diatomic molecule is given by

$$E_J = \frac{\hbar^2}{2\mathcal{I}} J(J+1), \qquad J = 0, 1, 2, \ldots,$$

where

$$\mathcal{I} = \frac{m_1 m_2}{m_1 + m_2} a^2$$

is the moment of inertia for masses m_1 and m_2 separated by a distance a.

(a) Sketch an energy level diagram for the vibration states $v = 0$ (ground state) and $v = 1$ and the rotation states $J = 0, 1, 2$. Use your sketch to indicate approximately the relative spacing of different energy levels and the allowed transitions between the $v = 0$ and $v = 1$ states for a molecule such as HCl. [20]

(b) Sketch the absorption spectrum resulting from the transitions in part (a). Indicate the relevant quantum numbers for the initial and final state of the transitions where possible. [20]

(c) Describe and explain how the spectrum in part (b) changes when the temperature of the gas is reduced. [20]

(d) The bond length in HCl is 0.127 nm. Estimate the frequency spacing between adjacent lines in the spectrum in part (b). [20]

(e) The HCl molecule is a *non-rigid rotator*. Describe and explain how this affects the appearance of the spectrum in part (b). [20]

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5. The vibrational energy of a diatomic molecule is given approximately by

$$E_v = \left(v + \frac{1}{2}\right)\hbar\omega_e$$

where $\omega_e = \sqrt{\frac{k}{\mu}}$, k is the bond force constant and μ is the reduced mass.

(a) Explain why this expression is an approximation and how a better estimate of the vibrational energy can be made. [20]

(b) Laser light with a wavelength of 632.1 nm scattered from F_2 gas at room temperature shows an emission line at 665.9 nm due to vibrational Raman scattering.

i. Estimate the bond force constant, k, for the F_2 molecule. [30]

ii. Explain why another line is seen near 602 nm and why this line is much weaker than the line at 665.9 nm. [20]

iii. Explain briefly what the existence of these Raman scattering lines implies for the polarizability of the F_2 molecule. [20]

(c) Explain why Raman scattering is particularly useful for studying molecules like F_2. [10]